

GENERALIZED BINOMIAL EDGE IDEALS

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ABSTRACT. This paper studies a class of binomial ideals associated to graphs with finite vertex sets. They generalize the binomial edge ideals, and they arise in the study of conditional independence ideals. A Gröbner basis can be computed by studying paths in the graph. Since these Gröbner bases are square-free, generalized binomial edge ideals are radical. To find the primary decomposition a combinatorial problem involving the connected components of subgraphs has to be solved. The irreducible components of the solution variety are all rational.

1. INTRODUCTION

Let X_0 and X_{in} be finite sets, $d_0 = |X_0| > 1$, and denote $X = X_0 \times X_{\text{in}}$. Let \mathbb{K} be a field, and consider the polynomial ring $\mathfrak{R} = \mathbb{K}[p_x : x \in X]$ with $|X|$ unknowns p_x indexed by X . For all $i, j \in X_0$ and all $x, y \in X_{\text{in}}$ let

$$f_{xy}^{ij} = p_{ix}p_{jy} - p_{iy}p_{jx}.$$

For any graph G on X_{in} the ideal I_G in \mathfrak{R} generated by the binomials f_{xy}^{ij} for all $i, j \in X_0$ and all edges (x, y) in G is called the d_0 th *binomial edge ideal* of G over \mathbb{K} . This is a direct generalization of [3] and [4], where the same ideals have been considered in the special case $d_0 = 2$. For a comparison of the results of the present paper to previous results see Remark 8.

One motivation to look at generalized binomial edge ideals comes from the study of conditional independence ideals. Given $n+1$ random variables X_0, X_1, \dots, X_n , generalized binomial edge ideals correspond to a collection of statements of the form (see [3] for an explanation of the notation and further details)

$$X_0 \perp\!\!\!\perp X_R | X_S = x_S,$$

where $R \cup S = \{1, \dots, n\}$. Such statements naturally occur in the study of robustness. Implications of the algebraic study of generalized binomial edge ideals will be studied in another paper [5], see also [3, Section 4]. Generalized binomial edge ideals also cover the conditional independence ideals associated with the intersection axiom in [2]. A different generalization of the results in [2] was recently studied in [7]. The ideals $I^{(1)}$ defined in [7] are special cases of binomial edge ideal.

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2. THE GRÖBNER BASIS

Choose a total order $>$ on \mathcal{X}_{in} (e.g. choose a bijection $\mathcal{X}_{\text{in}} \cong [N]$). This induces a lexicographic monomial order on \mathfrak{R} , also denoted by $>$, via

$$p_{ix} > p_{jy} \iff \begin{cases} \text{either} & i > j, \\ \text{or} & i = j \text{ and } x > y. \end{cases}$$

To construct a Gröbner basis for I_G with respect to this order the following definitions are needed:

Definition 1. A path $\pi : x = x_0, x_1, \dots, x_r = y$ from x to y in G is called *admissible* if

- (i) $x_s \neq x_t$ for $s \neq t$, and $x < y$;
- (ii) for each $k = 1, \dots, r-1$ either $x_k < x$ or $x_k > y$;
- (iii) for any proper subset $\{y_1, \dots, y_s\}$ of $\{x_1, \dots, x_{r-1}\}$, the sequence x, y_1, \dots, y_s, y is not a path.

A function $\kappa : \{0, \dots, r\} \rightarrow [d]$ is called π -*antitone* if it satisfies

$$x_s < x_t \implies \kappa(s) \geq \kappa(t), \text{ for all } 0 \leq s, t \leq r.$$

κ is *strictly π -antitone* if it is π -antitone and satisfies $\kappa(0) > \kappa(r)$.

The notion of π -antitonicity also applies to paths which are not necessarily admissible. However, since admissible paths are *injective* (i.e. they only pass at most once at each vertex), in the admissible case it is possible to write $\kappa(\ell)$ instead of $\kappa(s)$, if $\ell = x_s$.

To any $x < y$, any path $\pi : x = x_0, x_1, \dots, x_r = y$ from x to y and any function $\kappa : \{0, \dots, r\} \rightarrow \mathcal{X}_0$ associate the monomial

$$u_\pi^\kappa = \prod_{k=1}^{r-1} p_{\kappa(k)x_k}.$$

Theorem 2. *The set of binomials*

$$\mathcal{G} = \bigcup_{i < j} \left\{ u_{\pi f_{xy}}^{\kappa(y)\kappa(x)} : \begin{array}{l} x < y, \pi \text{ is an admissible path in } G \text{ from } x \text{ to } y, \\ \kappa \text{ is strictly } \pi\text{-antitone} \end{array} \right\}$$

is a reduced Gröbner basis of I_G with respect to the monomial order introduced above.

The role of π -antitonicity is the following: In smaller monomials $\prod_{k=1}^r p_{i_k x_k}$, smaller indices i_k are associated to larger points x_k . Hence the initial term of $u_{\pi f_{xy}}^{\kappa(y)\kappa(x)}$ is $u_\pi^\kappa p_{\kappa(y)x} p_{\kappa(x)y}$. This explains why in the definition of \mathcal{G} the point x is associated to the index $\kappa(y)$, and vice versa. The main idea of the proof of Theorem 2 is that reduction modulo \mathcal{G} changes the association of the indices $\{i_k\}$ and the points $\{x_k\}$ until the resulting monomial is minimal. The following lemma is a first step:

Lemma 3. *Let $\pi : x_0, \dots, x_r$ be a path in G , and let $\kappa : \{0, \dots, r\} \rightarrow [d]$ be an arbitrary function. If κ is not π -antitone, then there exists $g \in \mathcal{G}$ such that $\text{ini}_<(g)$ divides the initial term of $u_{\pi f_{xy}}^{\kappa(y)\kappa(x)}$.*

Proof. Let $\tau : y_0, \dots, y_s$ be a minimal subpath of π with respect to the property that the restriction of κ to τ is not τ -antitone. This means that κ is τ_0 -antitone and τ_s -antitone, where $\tau_0 = y_1, \dots, y_s$ and $\tau_s = y_0, \dots, y_{s-1}$. Assume without loss of generality that $y_0 < y_s$, otherwise reverse τ . The minimality implies that $\kappa(y_0) < \kappa(y_s)$. It follows that

τ is admissible: By minimality, if $y_0 < y_k < y_s$, then $\kappa(y_k) \geq \kappa(y_s) > \kappa(y_0) \geq \kappa(y_k)$, a contradiction. Define

$$\tilde{\kappa}(k) = \begin{cases} \kappa(s), & \text{if } k = 0, \\ \kappa(0), & \text{if } k = s, \\ \kappa(k), & \text{if } 0 < k < s. \end{cases}$$

Then $\tilde{\kappa}$ is τ -antitone, and $\text{ini}_{<}(u_{\tau}^{\tilde{\kappa}} f_{y_0 y_s}^{\tilde{\kappa}(y_s) \tilde{\kappa}(y_0)})$ divides $\text{ini}_{<}(u_{\pi}^{\tilde{\kappa}} f_{xy}^{\tilde{\kappa}(y) \tilde{\kappa}(x)})$. \square

Proof of Theorem 2. The proof is organized in three steps.

Step 1: \mathcal{G} is a subset of I_G . Let $\pi : x = x_0, x_1, \dots, x_{r-1}, x_r = y$ be an admissible path in G . The proof that $u_{\pi}^{\kappa} f_{xy}^{\kappa(j) \kappa(i)}$ belongs to I_G is by induction on r . Clearly the assertion is true if $r = 1$, so assume $r > 1$. Let $A = \{x_k : x_k < x\}$ and $B = \{x_\ell : x_\ell > y\}$. Then either $A \neq \emptyset$ or $B \neq \emptyset$.

Suppose $A \neq \emptyset$ and set $x_k = \max A$. The two paths $\pi_1 : x_k, x_{k-1}, \dots, x_1, x_0 = x$ and $\pi_2 : x_k, x_{k+1}, \dots, x_{r-1}, x_r = y$ in G are admissible. Let κ_1 and κ_2 be the restrictions of κ to π_1 and π_2 . Let $a = \kappa(r)$, $b = \kappa(0)$ and $c = \kappa(k)$. The calculation

$$\begin{aligned} & (p_{by} p_{ax} - p_{bx} p_{ay}) p_{cx_k} \\ &= (p_{bx_k} p_{cx} - p_{bx} p_{cx_k}) p_{ay} + (p_{ax_k} p_{by} - p_{ay} p_{bx_k}) p_{cx} - (p_{ax_k} p_{cx} - p_{ax} p_{cx_k}) p_{by} \end{aligned}$$

implies that $u_{\pi}^{\kappa} f_{xy}^{ab}$ lies in the ideal generated by $u_{\pi_1}^{\kappa_1} f_{x_k x}^{bc}$, $u_{\pi_2}^{\kappa_2} f_{x_k y}^{ab}$ and $u_{\pi_1}^{\kappa_1} f_{x_k x}^{ac}$. By induction it lies in I_G . The case $B \neq \emptyset$ can be treated similarly.

Step 2: \mathcal{G} is a Gröbner basis of I_G . Let $\pi : x_0, \dots, x_r$ and $\sigma : y_0, \dots, y_s$ be admissible paths in G with $x_0 < x_r$ and $y_0 < y_s$, and let κ and μ be π - and σ -antitone. By Buchberger's criterion it suffices to show that the S -pairs $S := S(u_{\pi}^{\kappa} f_{x_0 x_r}^{\kappa(r) \kappa(0)}, u_{\sigma}^{\mu} f_{y_0 y_s}^{\mu(s) \mu(0)})$ reduces to zero.

If $S \neq 0$, then S is a binomial. Write $S = S_1 - S_2$, where $S_1 = \text{ini}_{<}(S)$. S is homogeneous with respect to the multidegrees given by

$$\deg(p_{ix})_j = \delta_{ij} = \begin{cases} 1, & \text{if } i = j, \\ 0, & \text{else,} \end{cases}$$

and

$$\deg(p_{ix})_y = \delta_{xy} = \begin{cases} 1, & \text{if } x = y, \\ 0, & \text{else} \end{cases}$$

(this is a multidegree with $|\mathcal{X}_0| + |\mathcal{X}_{\text{in}}|$ components).

If π and σ are disjoint paths, then S trivially reduces to zero, since $u_{\pi}^{\kappa} f_{x_0 x_r}^{\kappa(r) \kappa(0)}$ and $u_{\sigma}^{\mu} f_{y_0 y_s}^{\mu(s) \mu(0)}$ contain different variables. So assume that π and σ meet and that $S \neq 0$. Then S_1 and S_2 are monomials, and the unknowns p_{ix} occurring in S_1 and S_2 satisfy $x \in \pi \cup \sigma$. Assume that there are $x < y$ such that $D_x := \min\{i \in \mathcal{X}_0 : p_{ix} | S_1\} < \max\{i \in \mathcal{X}_0 : p_{iy} | S_1\} =: D_y$. Since $\pi \cup \sigma$ is connected there is an injective path $\tau : z_0, \dots, z_s$ from $x = z_0$ to $y = z_s$ in $\pi \cup \sigma$. Choose a map $\lambda : \{0, \dots, s\} \rightarrow \mathcal{X}_0$ such that $\lambda(0) = D_x$, $\lambda(s) = D_y$ and $p_{\lambda(a)a} | S_1$ for all $0 \leq a \leq s$. Then u_{τ}^{λ} divides S_1 , and λ is not τ -antitone. So Lemma 3 applies, and S can be reduced to a smaller binomial.

Let S' be the reduction of S modulo \mathcal{G} . If $S' \neq 0$, then let $S'_1 = \text{ini}_{<}(S')$. The above argument shows that $\min\{i \in \mathcal{X}_0 : p_{ix} | S'_1\} \geq \max\{i \in \mathcal{X}_0 : p_{iy} | S'_1\}$ for all $x < y$. This property characterizes S'_1 as the unique minimal monomial in \mathfrak{R} with multidegree

$\deg(S'_1) = \deg(S)$. But since the reduction algorithm turns binomials into binomials, $S' - S'_1$ is also a monomial of multidegree $\deg(S)$, and smaller than $\deg(S'_1)$. This contradiction shows $S' = 0$.

Step 3: \mathcal{G} is reduced. Let $\pi : x_0, \dots, x_r$ and $\sigma : y_0, \dots, y_s$ be admissible paths in G with $x_0 < x_r$ and $y_0 < y_s$, and let κ and μ be π - and σ -antitone. Suppose that $u_\pi^\kappa p_{\kappa(r)x_0} p_{\kappa(0)x_r}$ divides either $u_\sigma^\mu p_{\mu(s)y_0} p_{\mu(0)y_s}$ or $u_\sigma^\mu p_{\mu(s)y_s} p_{\mu(0)y_0}$. Then $\{x_0, \dots, x_r\}$ is a subset of $\{y_0, \dots, y_s\}$, and $\kappa(b) = \mu(\sigma^{-1}(x_b))$ for $0 < b < r$. From admissibility follows $x_0 \leq y_0 < y_s \leq x_r$ and $\kappa(0) \geq \mu(0) > \mu(s) \geq \kappa(r)$.

If $x_0 < y_0$, then $p_{\kappa(r)x_0}$ divides u_σ^μ , and so $x_0 = y_t$ for some $t < s$ with $\mu(t) = u = \kappa(r)$. On the other hand, since $y_t \leq y_0$, it follows that $\mu(t) \geq \mu(0) > \kappa(r)$, a contradiction. Hence $x_0 = y_0$. Similarly, by a symmetric argument, $x_r = y_s$. This means that π is a sub-path of σ . By Definition 1, π equals σ . Therefore, $u_\pi^\kappa f_{x_0 x_r}^{\kappa(r)\kappa(0)}$ and $u_\sigma^\mu f_{y_0 y_s}^{\mu(s)\mu(0)}$ have the same (total) degree, and hence they agree. \square

Corollary 4. I_G is a radical ideal.

Proof. The assertion follows from Theorem 2 and the following general fact: A homogeneous ideal that has a Gröbner basis with square-free initial terms is radical. See the proof of [3, Corollary 2.2] for details. \square

3. THE PRIMARY DECOMPOSITION

Since I_G is radical, in order to compute the primary decomposition of the ideal it is enough to compute the minimal primes. From this it will be easy to deduce the irreducible decomposition of the variety V_G of I_G in the case of characteristic zero. The following definition is needed: Two vectors v, w (living in the same \mathbb{K} -vector space) are *proportional* whenever $v = \lambda w$ or $w = \lambda v$ for some $\lambda \in \mathbb{K}$. A set of vectors is *proportional* if each pair is proportional. Since $\lambda = 0$ is allowed, proportionality is not transitive: If v and w are proportional and if u and v are proportional, then u and w need not be proportional, because v may vanish.

Let V_G be the variety of I_G , which is a subset of $\mathbb{K}^{X_0 \times X_{\text{in}}}$. As usual, elements of $\mathbb{K}^{X_0 \times X_{\text{in}}}$ will be denoted with the same symbol $p = (p_{ix})_{i \in X_0, x \in X_{\text{in}}}$ as the unknowns in the polynomial ring $\mathfrak{R} = \mathbb{K}[p_{ix} : (i, x) \in X_0 \times X_{\text{in}}]$. Any $p \in \mathbb{K}^{X_0 \times X_{\text{in}}}$ can be written as a $d_0 \times |X_{\text{in}}|$ -matrix. Each binomial equation in I_G imposes conditions on this matrix saying that certain submatrices have rank 1. For a fixed edge (x, y) in G the equations $f_{xy}^{ij} = 0$ for all $i, j \in X_0$ require that the submatrix $(p_{kz})_{k \in X_0, z \in \{x, y\}}$ has rank one. More generally, if $K \subseteq G$ is a clique (i.e. a complete subgraph), then the submatrix $(p_{kz})_{k \in X_0, z \in K}$ has rank one. This means that all columns of this submatrix are proportional. The columns of p will be denoted by \tilde{p}_x , $x \in X_{\text{in}}$. A point p lies in V_G if and only if \tilde{p}_x and \tilde{p}_y are proportional for all edges (x, y) of G .

Even if the graph G is connected, not all columns \tilde{p}_x must be proportional to each other, since proportionality is not a transitive relation. Instead, there are “blocks” of columns such that all columns within one block are proportional. For any subset $\mathcal{Y} \subseteq X_{\text{in}}$ denote by $G_{\mathcal{Y}}$ the subgraph of G induced by \mathcal{Y} . Then:

- A point p lies in V_G if and only if \tilde{p}_x and \tilde{p}_y are proportional whenever $x, y \in \mathcal{S}$ lie in the same connected component of $G_{\mathcal{S}}$, where $\mathcal{S} = \{x \in X_{\text{in}} : \tilde{p}_x \neq 0\}$.

Let $V_{G, \mathcal{Y}}$ be the set of all $p \in \mathbb{K}^{X_0 \times X_{\text{in}}}$ for which $\tilde{p}_x = 0$ for all $x \in X_{\text{in}} \setminus \mathcal{Y}$ and for which \tilde{p}_x and \tilde{p}_y are proportional whenever $x, y \in X_{\text{in}}$ lie in the same connected

component of $G_{\mathcal{Y}}$. Then

$$(1) \quad V_G = \bigcup_{\mathcal{Y} \subseteq X_{\text{in}}} V_{G,\mathcal{Y}}.$$

The sets $V_{G,\mathcal{Y}}$ are rational irreducible algebraic varieties:

Lemma 5. *For any $\mathcal{Y} \subseteq X_{\text{in}}$ the set $V_{G,\mathcal{Y}}$ is the variety of the ideal $I_{G,\mathcal{Y}}$ generated by the monomials*

$$(2) \quad p_{ix} \quad \text{for all } x \in X_{\text{in}} \setminus \mathcal{Y} \text{ and } i \in X_0,$$

and the binomials f_{xy}^{ij} for all $i, j \in X_0$ and all $x, y \in \mathcal{Y}$ that lie in the same connected component of $G_{\mathcal{Y}}$. The ideal $I_{G,\mathcal{Y}}$ is prime, and the variety $V_{G,\mathcal{Y}}$ is rational.

Proof. The first statement follows from the definition of $V_{G,\mathcal{Y}}$. Write $I_{G,\mathcal{Y}}^1$ for the ideal generated by all monomials (2), and for any $\mathcal{Z} \subseteq \mathcal{Y}$ write $I_{\mathcal{Z}}^2$ for the ideal generated by the binomials f_{xy}^{ij} , with $i, j \in X_0$ and $x, y \in \mathcal{Z}$. Then $I_{G,\mathcal{Y}}^1$ is obviously prime. Each of the $I_{\mathcal{Z}}^2$ is a 2×2 determinantal ideal. It is a classical (but difficult) result that this ideal is the defining ideal of a Segre embedding, and that it is prime (see [6] for a rather modern proof). In fact, both $I_{G,\mathcal{Y}}^1$ and $I_{\mathcal{Z}}^2$ are geometrically prime, i.e. they remain prime over any field extension. Hence the ideal $I_{G,\mathcal{Y}}$ is the sum of the geometrically prime ideals $I_{G,\mathcal{Y}}^1$ and $I_{\mathcal{Z}}^2$ for all connected components \mathcal{Z} of $G_{\mathcal{Y}}$, and since the defining equations of all these ideals involve disjoint sets of unknowns, $I_{G,\mathcal{Y}}$ itself is prime. $V_{G,\mathcal{Y}}$ is rational, since the varieties of $I_{G,\mathcal{Y}}^1$ and $I_{\mathcal{Z}}^2$ are rational. \square

The decomposition (1) is not the irreducible decomposition of V_G , because the union is redundant. The redundant components can be removed using Lemma 5:

Lemma 6. *Let $\mathcal{Y}, \mathcal{Z} \subseteq X_{\text{in}}$. Then $V_{G,\mathcal{Y}}$ is contained in $V_{G,\mathcal{Z}}$ if and only if the following two conditions are satisfied:*

- $\mathcal{Y} \subseteq \mathcal{Z}$.
- If $x, y \in \mathcal{Y}$ are connected in $G_{\mathcal{Z}}$, then they are connected in $G_{\mathcal{Y}}$.

Proof. Assume that $V_{G,\mathcal{Y}} \subseteq V_{G,\mathcal{Z}}$. Then $I_{G,\mathcal{Y}} \supseteq I_{G,\mathcal{Z}}$. For any $x \in X_{\text{in}} \setminus \mathcal{Z}$ and any $i \in X_0$ this implies $p_{ix} \in I_{G,\mathcal{Y}}$. On the other hand, Lemma 5 shows that the point with coordinates

$$p_{iy} = \begin{cases} 1, & \text{if } y \in \mathcal{Y}, \\ 0, & \text{else,} \end{cases}$$

lies in $V_{G,\mathcal{Y}}$ and hence in $V_{G,\mathcal{Z}}$. This implies $x \in X_{\text{in}} \setminus \mathcal{Y}$; and so $\mathcal{Y} \subseteq \mathcal{Z}$.

Let $x \in \mathcal{Y}$. Choose two linearly independent non-zero vectors $v, w \in \mathbb{K}^{d_0}$. By Lemma 5 the matrix with columns

$$\tilde{p}_y = \begin{cases} v, & \text{if } y \in \mathcal{Y} \text{ is connected to } x \text{ in } G_{\mathcal{Y}}, \\ w, & \text{if } y \in \mathcal{Y} \text{ is not connected to } x \text{ in } G_{\mathcal{Y}}, \\ 0, & \text{else,} \end{cases}$$

is contained in $V_{G,\mathcal{Y}}$ and hence in $V_{G,\mathcal{Z}}$. Therefore, if z is connected to x in $G_{\mathcal{Z}}$, then it is connected to x in $G_{\mathcal{Y}}$.

Conversely, if both conditions are satisfied, then all defining equations of $I_{G,\mathcal{Z}}$ lie in $I_{G,\mathcal{Y}}$. \square

Theorem 7. *The primary decomposition of V_G is $I_G = \bigcap_{\mathcal{Y}} I_{G,\mathcal{Y}}$, where the intersection is over all $\mathcal{Y} \subseteq X_{\text{in}}$ such that the following holds: For any $x \in X_{\text{in}} \setminus \mathcal{Y}$ there are edges $(x, y), (x, z)$ in G such that $y, z \in \mathcal{Y}$ are not connected in $G_{\mathcal{Y}}$. Equivalently, for any $x \in X_{\text{in}} \setminus \mathcal{Y}$ the induced subgraph $G_{\mathcal{Y} \cup \{x\}}$ has fewer connected components than $G_{\mathcal{Y}}$.*

Proof. First, assume that \mathbb{K} is algebraically closed. By (1) and Lemma 5 it suffices to show that the condition on \mathcal{Y} stated in the theorem characterizes the maximal sets $V_{G,\mathcal{Y}}$ in the union (1) (with respect to inclusion). This follows from Lemma 6.

If \mathbb{K} is not algebraically closed, then one can argue as follows: By [1] a binomial ideal has a binomial primary decomposition over some algebraic extension field $\bar{\mathbb{K}} = \mathbb{K}[\alpha_1, \dots, \alpha_k]$. The algebraic numbers $\alpha_1, \dots, \alpha_k$ are coefficients of the defining equations of the primary components. Let $\bar{\mathbb{K}}$ be the algebraic closure of \mathbb{K} . Since the ideals $I_{G,\mathcal{Y}}$ are defined by pure differences and since the ideals $\bar{\mathbb{K}} \otimes I_{G,\mathcal{Y}}$ are the primary components of $\bar{\mathbb{K}} \otimes I_G$ in $\bar{\mathbb{K}} \otimes \mathbb{R}$ it follows that the ideals $I_{G,\mathcal{Y}}$ are already the primary components of I_G (in other words, the primary decomposition is independent of the base field). \square

Remark 8 (Comparison to [4, 3]). Both [4] and [3] discuss Gröbner bases and primary decompositions of binomial edge ideals with $d_0 = 2$. Theorem 2 generalizes Theorems 2.1 from [3] and Theorem 3.2 in [4]. While the proofs in [3] and [4] use a case by case analysis, the proof of Theorem 2 is more conceptual.

The primary decomposition in Theorem 7 generalizes Theorem 3.2 from [3]. The proof of Theorem 7 relied on the irreducible decomposition of the corresponding variety, while the proof in [3] directly shows the equality of the two ideals.

Instead of describing the primary decomposition explicitly, [4] presents an algorithm to compute the primary decomposition. Since the primary decomposition of a binomial edge ideal is independent of d_0 , the same algorithm applies for all d_0 . A nice feature of the algorithm is that it works graph-theoretically.

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